WO 2005/087777 PCT/KR2004/000536

What is claimed is:

1. A disubstituted cucurbit[m]uril where m is 5 to 8, represented by the following Formula 1:

$$\begin{array}{c|c}
X \\
N-CH_2 \\
R \\
N-CH_2
\end{array}$$

$$\begin{array}{c|c}
N - CH_2 \\
H \\
N - CH_2
\end{array}$$

$$\begin{array}{c|c}
N - CH_2 \\
N - CH_2
\end{array}$$

$$\begin{array}{c|c}
N - CH_2 \\
N - CH_2
\end{array}$$

$$\begin{array}{c|c}
N - CH_2 \\
N - CH_2
\end{array}$$

wherein n is an integer of 4 to 7;

X is O, S, or NH;

R is selected from the group consisting of a substituted or unsubstituted alkenyl group of C2-C30, a substituted or unsubstituted alkylcarboxyl group of C1-C30, a substituted or unsubstituted alkylcarboxyl group of C1-C30, a substituted or unsubstituted hydroxyalkyl group of C1-C30, a substituted or unsubstituted alkoxy group of C1-C30, a substituted or unsubstituted heteroaryl group of C6-C30.

15

20

25

10

5

- 2. The disubstituted cucurbit[m]uril of claim 1, wherein R is selected from the group consisting of a 2-nitrophenyl group, a 3-nitrophenyl group, a 4-nitrophenyl group, a 2-methoxyphenyl group, a 3-methoxyphenyl group, a 4-methoxyphenyl group, a 2-aminophenyl group, a 3-aminophenyl group, a 4-aminophenyl group, a 2-hydroxyphenyl group, a 3-hydroxyphenyl group, and a 4-hydroxyphenyl group.
- 3. The disubstituted cucurbit[m]uril of claim 1 or 2, which is used as column packing materials for chromatography, additives to gas separation membranes, catalysts for various chemical reactions, chemical sensors, biological sensors, or drug carriers.

WO 2005/087777 PCT/KR2004/000536

4. A method for preparing a disubstituted cucurbituril represented by Formula 1, comprising reacting a disubstituted glycoluril represented by Formula 2 and a glycoluril represented by Formula 3 with formaldehyde:

$$\begin{array}{c|c}
 & X \\
 & N - CH_2 \\
 & R \\
 & N - CH_2 \\
 & N - CH_2 \\
 & N - CH_2
\end{array}$$

$$\begin{array}{c|c}
 & N - CH_2 \\
 & N - CH_2 \\
 & N - CH_2
\end{array}$$

$$\begin{array}{c|c}
 & N - CH_2 \\
 & N - CH_2
\end{array}$$

$$\begin{array}{c|c}
 & N - CH_2 \\
 & N - CH_2
\end{array}$$

$$\begin{array}{c|c}
 & N - CH_2 \\
 & N - CH_2
\end{array}$$

$$\begin{array}{c|c}
 & N - CH_2 \\
 & N - CH_2
\end{array}$$

$$\begin{array}{c|c}
 & N - CH_2
\end{array}$$

5

10

15

20

(2) HN NH H HN NH

wherein n is an integer of 4 to 7;

X is O, S, or NH;

R is selected from the group consisting of a substituted or unsubstituted alkenyl group of C2-C30, a substituted or unsubstituted alkylcarboxyl group of C2-C30, a substituted or unsubstituted alkylcarboxyl group of C2-C30, a substituted or unsubstituted hydroxyalkyl group of C1-C30, a substituted or unsubstituted alkoxy group of C1-C30, a substituted or unsubstituted aryl group of C6-C30, and a substituted or unsubstituted heteroaryl group of C6-C30.

5. The method of claim 4, wherein the disubstituted glycoluril of Formula 2 is prepared by reacting a 1,2-diketone derivative represented by

WO 2005/087777

5

15

20

25

30

Formula 4 with an urea represented by Formula 5 in the presence of an acid catalyst:

$$\begin{array}{c}
O & R \\
R & O
\end{array}$$

$$\begin{array}{c}
(4) \\
H_2N & NH_2
\end{array}$$

(5)

wherein X and R are as defined in claim 4.

- 6. The method of claim 5, wherein the acid catalyst is one or more selected from the group consisting of a hydrochloric acid, a sulfuric acid, and a trifluoroacetic acid.
 - 7. The method of claim 5, wherein the acid catalyst is primarily added and stirred at 70-85°C for 20-60 minutes and, when gelation occurs, the acid catalyst is further added and stirred at 90-100°C for 12-30 hours.
 - 8. The method of claim 5, wherein after the reaction, a resultant solution is left stand at room temperature for 1-20 hours and a cucurbituril precipitate is filtrated to obtain a disubstituted cucurbituril-containing filtrate.
 - 9. The method of claim 8, wherein one or more of acetone and methanol is added to the filtrate to form a precipitate and the precipitate is washed with a mixed solvent of acetone and water in a volume ratio of 2:1 to 10:1 to prepare the disubstituted cucurbituril of Formula 1.
 - 10. The method of claim 4, wherein the disubstituted cucurbituril of Formula 1 where R is an aminophenyl group is prepared by reacting the disubstituted glycoluril of Formula 2 where R is a nitrophenyl group and the glycoluril of Formula 3 with the formaldehyde to form a disubstituted cucurbituril of Formula 1 where R is an nitrophenyl group, followed by reduction of the

WO 2005/087777 PCT/KR2004/000536

disubstituted cucurbituril of Formula 1 where R is an nitrophenyl group.

5

10

15

20

11. The method of claim 10, wherein the reduction is carried out in the presence of one or more reducing agents selected from the group consisting of hydrogen, ammonium formate, tin and tin chloride, hydrazine, iron and iron chloride, zinc, formic acid, hydrogen sulfide, ammonia, sodium sulfide, titanium chloride, and aqueous ammonium sulfide solution.

- 12. The method of claim 4, wherein the disubstituted cucurbituril of Formula 1 where R is a hydroxyphenyl group is prepared by reacting the disubstituted glycoluril of Formula 2 where R is a methoxyphenyl group and the glycoluril of Formula 3 with the formaldehyde to form a disubstituted cucurbituril of Formula 1 where R is an methoxyphenyl group, followed by deprotection of the disubstituted cucurbituril of Formula 1 where R is an methoxyphenyl group.
- 13. The method of claim 12, wherein the deprotection is carried out in the presence of one or more selected from the group consisting of boron tribromide, boron trichloride, sodium alkyl sulfide, sodium sulfide, sodiumcyanide, lithium iodide, aluminum bromide, 9-BBN, pyridinium chloride, methyl magnesium iodide, hydrobromic acid, acetic acid, aluminum chloride, and lithium chloride.